517,739

(12) INTERNATIONAL APPLICATION PUBLISHED UNDER THE PATENT COOPERATION TREATY (PCT)

(19) World Intellectual Property Organization
International Bureau

(43) International Publication Date
24 December 2003 (24.12.2003)

PCT

(10) International Publication Number
WO 03/107120 A2

(51) International Patent Classification[7]: G06F

(21) International Application Number: PCT/US03/18218

(22) International Filing Date: 12 June 2003 (12.06.2003)

(25) Filing Language: English

(26) Publication Language: English

(30) Priority Data:
60/387,953 13 June 2002 (13.06.2002) US

(71) Applicant *(for all designated States except US)*: **3-DIMENSIONAL PHARMACEUTICALS, INC.** [US/US]; Three Lower Makefield Corporate Center, 1020 Stony Hill Road, Suite 300, Yardley, PA 19067 (US).

(72) Inventors; and

(75) Inventors/Applicants *(for US only)*: **AGRAFIOTIS, Dimitris, K.** [US/US]; 660 Perimiter Drive, Downington, PA 19335 (US). **XU, Huafeng** [CN/US]; 127H, The Orchard, 60 One Mile Road, Cranbury, NJ 08512 (US). **SALEMME, Francis, R.** [US/US]; 1970 Timber Lakes Drive, Yardley, PA 19067 (US).

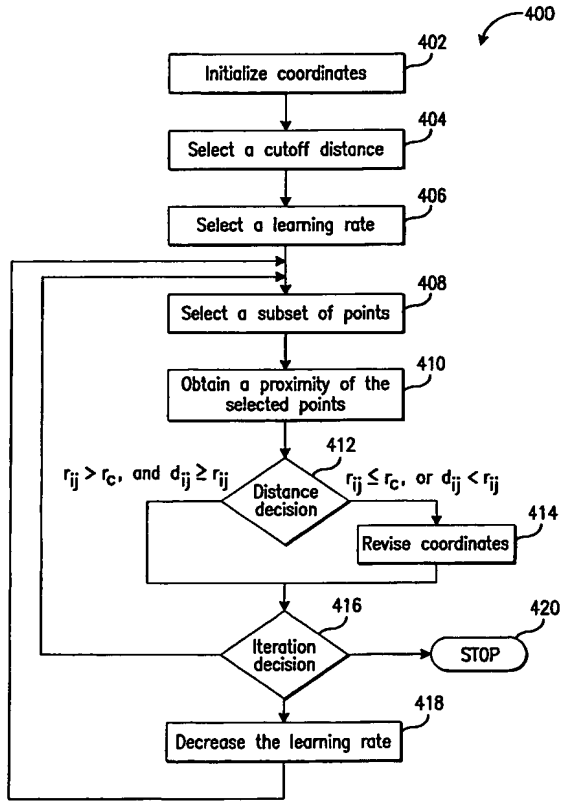
(74) Agents: **NORTON, Vicki, G.**, et al.; PILLSBURY WINTHROP, LLP, 11682 El Camino Real, Suite 200, San Diego, CA 92130-2092 (US).

(81) Designated States *(national)*: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW.

(84) Designated States *(regional)*: ARIPO patent (GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW),

[Continued on next page]

(54) Title: METHODS, SYSTEMS, AND COMPUTER PROGRAM PRODUCTS FOR REPRESENTING OBJECT RELATIONSHIPS IN A MULTIDIMENSIONAL SPACE



(57) Abstract: Methods, systems and computer program products for mapping a set of related objects into a multidimensional space. The mapping is carried out using an iterative (e.g., pairwise) refinement strategy that attempts to ensure that the distances of the objects on the map satisfy a supplied set of upper and lower bounds. In a preferred embodiment, these upper and lower bounds are derived from a supplied set of relationships (similarities, dissimilarities, or proximities) between the objects. In another preferred embodiment, these distance bounds are chosen to preserve local relationships between neighboring objects while maintaining minimum separation between remote objects.

WO 03/107120 A2